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NUMERICAL PREDICTION OF THE DIFFUSION OF EXHAUST PRODUCTS OF SUPERSONIC AIRCRAFT IN THE STRATOSPHERE

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NUMERICAL PREDICTION OF THE DIFFUSION OF EXHAUST PRODUCTS OF SUPERSONIC AIRCRAFT IN THE STRATOSPHERE

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ABSTRACT. It is known that the contribution of air traffic to global air pollution has amounted to only a few tenths of a percent over the last few years and that the replacement of present day aircraft with supersonic aircraft will not greatly change this contribution. New atmospheric problems of high altitude flight appear to call for some new ideas, especially in the area of reactions and photochemical equilibria at the level of the ozonosphere. Also the behavior of water vapor in the stratosphere must be investigated. The aim of the present paper is to make a contribution to such predictions on a serious scientific basis. We begin by evaluating the diffusion of gaseous or finely scattered products (nitrogen oxides, carbon monoxide, water vapor) which can become suspended in the stratosphere. For this purpose, we will take advantage of the extensive experience of the French Atomic Energy Commission on the industrial level (lower atmospheric strata, small distance scale) as well as in the military applications area (for all altitudes, long period, large scale). Numerical results are given assuming three hundred supersonic jets, each making a return trip every day on a heavily traveled route.

PROBLEM FORMULATION /38*

Any human activity which involves energy transformations results in the release of by-products or wastes which can affect the integrity of the environment. In all cases, a compromise must be reached between the activity being pursued and the requirement for maintaining the integrity of the environment within tolerable limits.

*Numbers in the margin indicate pagination in the original foreign text.

As far as aerial commerce is concerned, it is necessary to take into account the complex interactions between the areas actually traversed and other parts of the atmosphere and biosphere.

The contribution of this activity to world pollution over the last few years does not exceed a few tenths of a percent. If part of the present day aircraft are replaced by supersonic aircraft, this contribution will not be greatly changed.

Nevertheless it is necessary to consider the new aspects of very high altitude flights, especially in particularly sensitive layers in which complex photochemical phenomena take place or where the material density is small. The equilibrium conditions, reactions and exchanges affect the biosphere down to the low layers (insulation, temperature, humidity, ultra-violet radiation).

In a general way, the introduction of certain products is not critical by itself, especially if these products are subject to dispersion processes. However, it is necessary to constantly monitor the modifications of the natural state and the long term accumulation of various types of pollutants.

We will first attempt to give a numerical evaluation of the maximum concentrations of nitrogen oxides, carbon dioxide and water vapor over ten years in the stratosphere. We will not take into account the dissociation and dispersion processes which are certainly present. We will assume 300 "Concorde" aircraft each perform a daily round trip over a heavily traveled air route.

To this first pessimistic evaluation, we can always apply dissociation and dispersion functions of time derived from special studies, so we can finally arrive at values which will be closer to reality.

METHOD OF APPROACH AND TREATMENT

General Remarks

The public first became concerned with damage to the integrity of the environment because of the nuclear explosions in Japan. This is probably why the greatest relative and absolute amounts of expenditures in the area of environmental integrity have been made in investigating nuclear activity.

This effort was directed in various directions. Vast amounts of money were spent for industrial applications, space applications and military applications. In other words, investigations were carried out at all levels, all scales and all "numbers".

Because of its long experience and its intimate knowledge with experience obtained in foreign countries, the French Atomic Energy Commission was looked upon as one of the most qualified organizations to participate in the solution of similar problems in which geophysical concepts of the less explored regions (low stratosphere) and the physics of gases and of aerosals were involved. In spite of the customary delays due to uncertainties, it was able to give solutions to these problems in a form that could be immediately exploited.

A recent publication of the Atomic Energy Commission (C.E.A.) [1] outlined the methodology for treating the actual problem of numerical prediction of the diffusion of exhaust products from commercial supersonic aircraft into the stratosphere.

This publication sets forth a very general solution which is valid for all types of fixed points or extended sources of gases or fine aerosols. It could be extended to various types of aerosols, if the dimensions of the particles (micron size or submicron size) are compatible with the natural turbulence scale which holds them in suspension and which provides for their diffusion.

This is a gaussian type solution of the partial differential equations of turbulent diffusion transfer of heat, momentum or matter. This amounts to assuming that a source which is a point or which is considered as a point will diffuse these quantities according to a normal three-dimensional law, with three standard deviations. This is in good agreement with what is observed in nature.

The compatibility conditions between the adopted solution and the initial diffusion equation of course imply that exact relationships between the standard deviations of the solution and the diffusion coefficients of the initial equation exist.

In this connection it should be noted that the diffusion coefficients used, /39
especially for transfer of momentum and matter, have been determined for gases and

have been verified using radioactive gas tracers (radon, tritium). This was then extended by experiments in which radioactive tracers, liquid aerosols and solids were used. The dimensions and the volumetric masses of the solids were subjected to certain conditions.

Of course an aircraft is not a fixed source, but a simple transformation can make it become one. In models it is sufficient to replace the average wind velocity by the vector sum of the average wind velocity and a vector which is equal and opposite to the velocity of the aircraft. Then the results which are directly obtained as a function of the distance behind each aircraft (continuous source and quasi-permanent conditions) are translated as a function of the elapsed time after each passage, taking the true velocity of the aircraft into account. These results always give information regarding the concentration of the expelled products and the dimensions of the polluted space.

For a short time, less than one day, the wakes of each aircraft are treated separately.

In the case where there is a continuous flow of heavy traffic, the cumulative effects are calculated at a central point as a function of the elapsed time beginning 24 hours after the beginning of traffic. The durations and times at which conditions return to normal after a hypothetical stop in the traffic are also calculated.

Analytical Techniques

The mathematical formulation used for the numerical calculations distinguishes three types of situations:

— a single aircraft, in which the four engines are assumed to be located at one point, or several aircraft flying in formation with distances between them such as they can all be considered as located at the same point;

— several aircraft passing through the same point at equal time intervals;

— several aircraft have passed through the same point at equal time intervals, and traffic has stopped since a predetermined time.

1 — The following is an expression for the concentration distribution of exhaust products in a given vertical plane, as a function of the elapsed time since the passage of the aircraft in this plane or the passage of a group of aircraft which can be considered as a single source:

$$\chi_1 = \int_{-\infty}^{t} \frac{\lambda Q \, dte}{(2\pi)^{3/2} \, \sigma_x \sigma_y \sigma_z} \cdot e^{-\frac{1}{2}\left[\frac{[|V|t - |U - V|(t - t_e)]^2}{\sigma_x^2} + \frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}\right]} \qquad (1)$$

with

$$\sigma_x = [A_x (t - t_e)]^{k_x} \qquad (2)$$

$$\sigma_y = [A_y (t - t_e)]^{k_y} \qquad (3)$$

$$\sigma_z = [A_z (t - t_e)]^{k_z} \qquad (4)$$

where:

χ_1	Volume concentration of the emitted gases or aerosols.
λQ	Emission flow rate.
t	Elapsed time since passage.
t_e	Time of emission of a gas or aerosol cloud calculated from the instant of passage.
$\sigma_x, \sigma_y, \sigma_z$	Standard deviations of the gases or the aerosols in the three directions of space measured from the wake axis.
A_i, k_i	Numerical coefficients which depend on the diffusion properties in the stratosphere [1].
V	Velocity vector of the aircraft with respect to the ground.
U	Velocity vector of the average wind (drift neglected).
y	Horizontal position coordinate in the direction perpendicular to the wake axis.
z	Vertical position coordinate with respect to the wake axis.

The lower limit of the interval of integration with respect to the time of emission, infinity, simply indicates that at a given point of the wake, i.e., at a fixed distance behind the aircraft, quasi-permanent conditions are assumed. At the same time, any possible recent variations in the emission flow rate which could lead to fluctuations are ignored.

Assuming that the effect of the wind is correctly taken into account for the calculation of the concentrations in equation (1), there nevertheless exists sinchronization and positioning problems which occur in the case where there is drift of the wake caused by a transverse wind.

If there is a headwind or a tailwind, these difficulties do not occur. This is what we will assume in this first approach. This simplification becomes more justified as we investigate the long-term cumulative effects.

2 — The expression for the concentration distribution of the exhaust products in a given vertical plane after passage of several aircraft or equally spaced groups of aircraft is given by the following as a function of passage frequency and the time which has elapsed since the first passage:

$$X_n(t) = X_1(t_o) + \frac{1}{\Delta t}\int_{t_o}^{t} X_1(t)\,dt \qquad (5)$$

with:

$$\Delta t = \frac{t - t_o}{n-1} \qquad (6)$$

and:

$$\Delta t \ll t - t_o \qquad (7)$$

where:

X_n (t)	Volumetric concentration after n passages over a time interval t.
X_1 (t_0)	Partial volumetric concentration due to the last passage after a time t_0 (we will always assume that $t_0 \neq 0$, such that we never have to consider theoretically infinite point concentrations).
Δt	Time interval between two passages.

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3 — Expression for the distribution of the concentrations of exhaust products in a given vertical plane after passage of several aircraft or groups of equally spaced aircraft, as a function of the passage frequency, the time elapsed between the first and the last passage and the time elapsed since the first passage:

$$X_n(t_a,t) = X_1(t_o+t-t_a) + \frac{1}{\Delta t}\int_{t_o+t-t_a}^{t} X_1(t)\,dt \qquad (8)$$

with:

$$\Delta t = \frac{t_a - t_o}{n-1} \qquad (9)$$

and:

$$\Delta t \ll t - t_o \tag{10}$$

where:

$\chi_n(t_a, t)$,	Volumetric concentration at the end of the time of n passages up to a time $t_a < t$.
$\chi_1(t_0+t-t_a)$	Partial volumetric concentration due to the last passage after a time $t_0 + (t-t_a)$.
Δt	Time interval between two passages.

Expressions (5) and (8) are obtained using conditions (7) and (10) by applying the averaging formula, derived from expression (1), to the problem of calculating cumulative concentrations due to the superposition of several identical plumes which are displaced in time by a constant amount.

RESULTS

Methods of Presentation

We will make the hypothesis that on a greatly traveled aerial route, 300 supersonic transports of the "Concorde" type each make a round trip lasting approximately 7 hours every 24 hours at an altitude of 16 kilometers. In addition, it is assumed that each pair of aircraft fly at the same altitude separated by a distance of 100 kilometers, and that the 600 trips are uniformly distributed over time. Under these conditions, if cumulative effects are of interest in all regions of space, it is sufficient to consider a line which is essentially perpendicular to the general direction of these flight paths. We may assume a continuous sequence of passes of four aircraft, two in each direction and every 576 seconds. This amounts to 150 passes every 24 hours. For each pass, a lateral uniform displacement of 100 kilometers for the four aircraft is assumed. The velocity is also assumed to be uniform and is equal to 600 meters per second.

The concentrations are specified in arbitrary units (for example, mass) per cubic meter of local air, for a unit output per aircraft in the same unit per second. Such a representation has the advantage of being independent of the unit which expresses the diffused substance. It has the dimension of time per volume, in this case seconds per meter of local air ($s.m^{-3}$). For any output, all the true concentrations are automatically obtained by simply multiplying by this output after verifying that the units agree.

The concept of the dimensions of the polluted space would strictly speaking have to be replaced by the concept of the concentration gradient of pollution in this space. It is known that the adopted model is used to predict the maximum probability that pollution products will be present in the immediate vicinity of the aircraft wakes. It is also used to predict the decreasing probabilities as one moves away from these wakes. Under these conditions, it is possible to establish a connection between the two contents which makes it possible to specify quantities, which have units of meters or kilometers, which specify the size of the horizontal space which contains a given proportion of the total contamination at a given time. This is done using the definition of the standard deviations. A similar reasoning also holds for the vertical dimension. The proportion adopted is 97% such that the indicated dimensions, equal to 4.3 σ, also equal twice the distance from the wake where the concentration amounts to only one tenth of the maximum value within the wake. It is also interesting to note that these particular features remain valid in the case where there are several parallel wakes, if the time periods are sufficiently long for the effects to accumulate, which means that the global distribution will have become normal itself.

"Unit" Numerical Values

Following the presentation methods mentioned above, we have collected the results of various calculations carried out on the machine using the same unit output in the five following tables.

Figure 1 shows the maximum concentration and the size in the wake of one aircraft for elapsed times from 10 seconds to 1 hour after its passage. During this time, the maximum concentration decreases from 10^{-3} to 10^{-9} $s.m^{-3}$, and the size increases from 1 meter to 10 kilometers.

Figure 2 shows the same information up to 24 hours, at which time the maximum concentration becomes less than 10^{-10} $s.m^{-3}$ and the size becomes 170 kilometers.

Figure 3 shows five concentration profiles along vertical sections perpendicular to the relative displacement with respect to the air, for elapsed times from 7 hours to 15 days after the passage of four aircraft which fly at the same velocity (600 $m.s^{-1}$) and at the same altitude, separated by a distance of 100 kilometers. The transition of the four normal distributions into one occurs during a

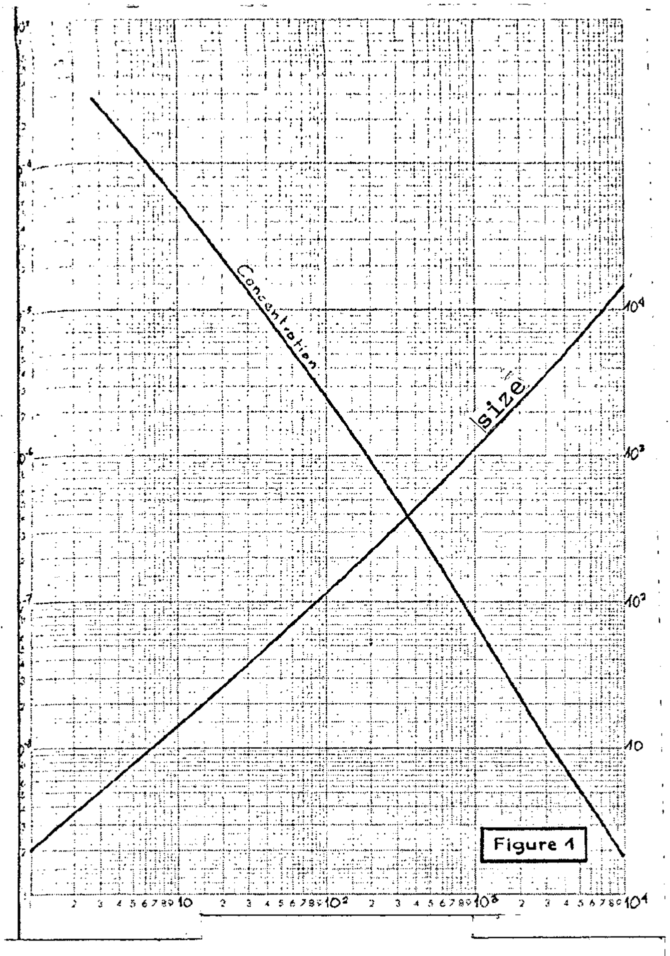

Fig. 1. Time in seconds.

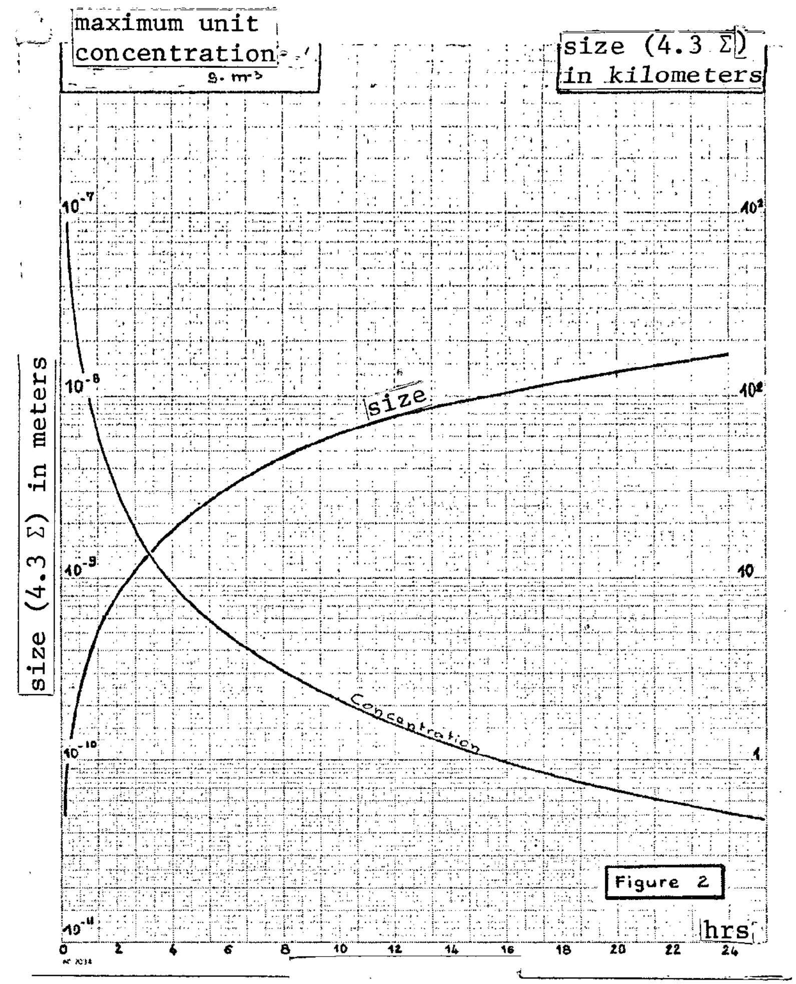

Fig. 2. Time in hours.

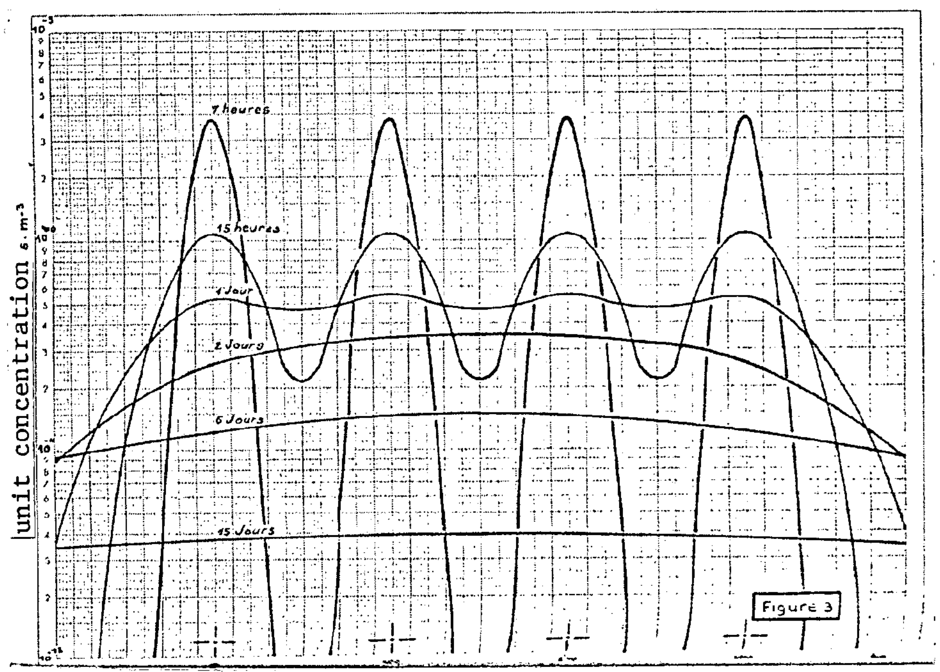

Fig. 3.

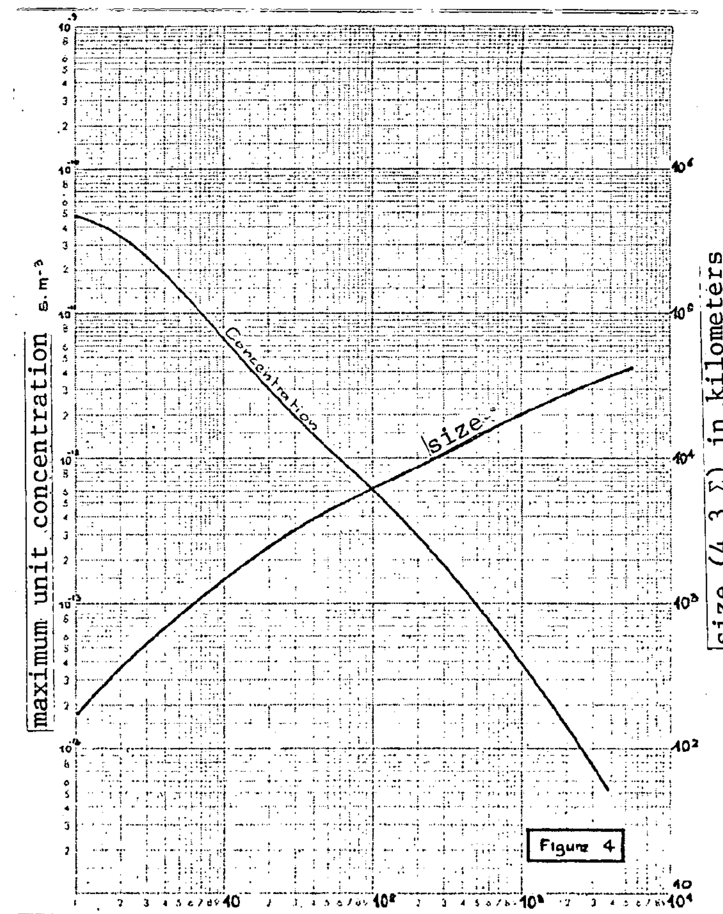

Fig. 4. Time in days.

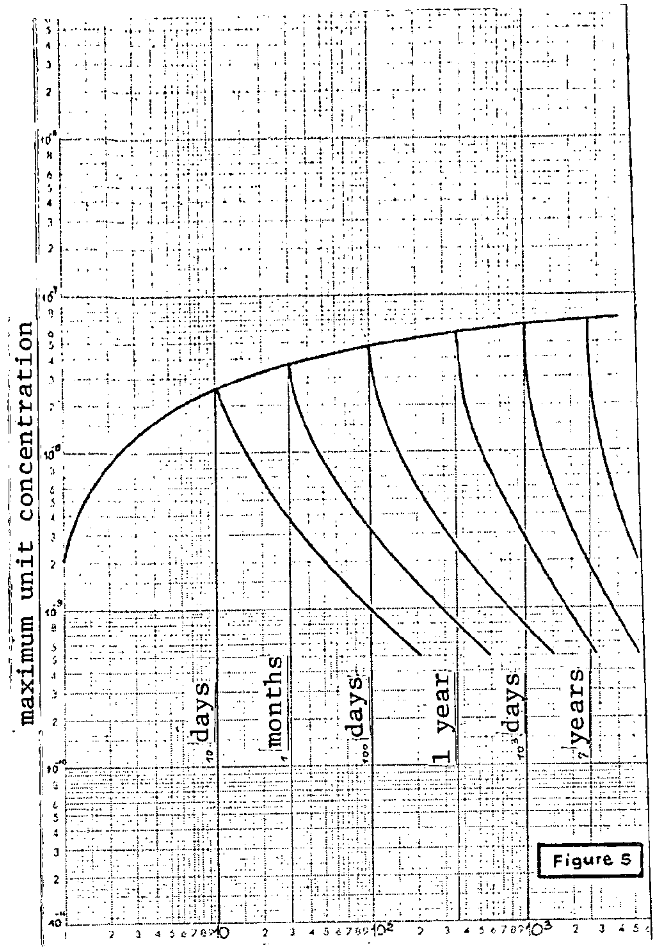

Fig. 5. Time in days.

transition phase at about 1 day. It is very clear in the figure. The maximum concentrations decrease /42 from 4.10^{-10} to 4.10^{-12} s.m^{-3} during the same time period and the sizes can be directly read off, at least up to 1 day, because these are complete profiles.

Figure 4 extends these data up to 10 years for an aircraft or a group of aircraft. It verifies the data given in the first two figures. The concentrations and the size in the wake of a single aircraft or a group of aircraft are given for elapsed times from 1 day to 10 years. During this long delay where on the average there is a large zone having small gradients, the probable maximum concentration decreases from 5.10^{-11} s.m^{-3} to 5.10^{-15} s.m^{-3}, and the order of magnitude of the space affected increases from 170 to 35,000 kilometers. This latter quantity only means that ten years after pollution has been initiated due to the theoretical flight of one aircraft or a group of aircraft, the pollution is diffused over an area on the scale of the earth and the concentrations are quasi-uniform.

The fifth and last figure shows final results corresponding to the entire problem considered here. This considers the traffic of 300 aircraft under the conditions mentioned above. This is the maximum cumulative concentration due to the passage of 300 aircraft, as a function of the duration of this traffic, which extends from 1 day to 10 years. It is assumed that this traffic stops 10 days to 7 years after after it is started. This cumulative concentration, which can be derived from the previous ones by the addition of numerous identical suitably displaced plumes, naturally will increase as a function of time. First it increases rather rapidly from 2.10^{-9} to 3.10^{-8} s.m^{-3} between 1 and 15 days, but then more slowly from 3.10^{-8} to 7.10^{-8} $s.m^{-3}$ between 15 days and 10 years, provided that the traffic is not interrupted.

Additional curves are shown in order to provide an idea of the return to normal conditions in case there is an interruption in the traffic. For example, that between 100 days and 4 years, there would be a concentration reduction by a factor of 100, which would essentially mean a return to the initial conditions. This return usually occurs after a delay on the order of 2 to 5 times the duration of the traffic.

Some Orders of Magnitude for the "Concorde"

The "Concorde" consumes 25 tons of fuel per hour.

On the other hand, during the third OACI Conference (Montreal, September-October 1971 [4]) estimates of the order of magnitude of the pollution emission indices were formulated and were matched with strict conditions, which the reader will remember [4].

The following table shows the estimates for the pollutants which must be considered. It gives some examples from the previous discussion of maximum concentrations which it could produce. Dissociation and dispersion processes are not considered. This is done assuming that a continuous traffic of 300 aircraft is uninterrupted after a certain time.

Pollutant	Emission index	Emission output	Maximum concentrations**	
			at 10 days $4.3\ \sigma = 1500$ km	at 10 years $4.3\ \sigma = 36000$ km
	grams per gram of fuel	$g.s^{-1}$	$g.m^{-3}$ (ppm*)	$g.m^{-3}$ (ppm*)
H_2O	1,3	$9{,}03.10^{3}$	$2{,}26.10^{-4}$ (1,13)	$6{,}34.10^{-4}$ (3,17)
NO	$1{,}25.10^{-2}$	86,5	$2{,}16.10^{-6}$ ($1{,}08.10^{-2}$)	$6{,}06.10^{-6}$ ($3{,}03.10^{-2}$)
CO	$3{,}7.10^{-3}$	25,7	$6{,}40.10^{-7}$ ($3{,}20.10^{-3}$)	$1{,}81.10^{-6}$ ($0{,}90.10^{-2}$)

*mass
**commas represent decimal points

If the diffused water vapor concentration is known as a function of time after the passage of an aircraft, i.e., as a function of the distance within its wake, we may at least theoretically calculate the dimensions of the areas in which vapor trails will probably be formed, provided that the specific humidity and the specific saturating humidity are known under the encountered atmospheric conditions. /43

It is difficult to obtain information regarding the specific saturating humidity (or the ratio of saturating mixture) in the stratosphere. Recent publications [2] and [3] give certain indications which can be summarized by means of the following table:

Ratio of saturating mixture at 100 mb (16 km)		
Temperature °C	Saturating concentration	Radio of saturating mixture
	$g.m^{-3}$	$g.g^{-1}$
– 39	2.10^{-1}	1.10^{-3}
– 45	1.10^{-1}	5.10^{-4}
– 58	2.10^{-2}	1.10^{-4}
– 62	1.10^{-2}	5.10^{-5}
– 72	2.10^{-3}	1.10^{-5}
– 78	1.10^{-3}	5.10^{-6}

The "unit" saturating concentration in $s.m^{-3}$ is determined from the ratio of the saturating mixture reduced by the natural content and translated into saturating concentration. Also the emission output per aircraft is used. From this the trail is calculated as a function of time since the aircraft made the pass. In other words, it is calculated as a function of the distance within the wake measured from the aircraft.

This estimate can be made using Figure 1. This is done by using known relationships between the distribution law and its standard deviation for each type of compound.

The following table summarizes some of these estimates for a natural content of 3.10^{-6} $g.g^{-1}$ [2], [3], and for four values of the saturating mixture ratio rs. These are most frequently encountered at medium latitudes in the stratosphere of the North Allantic, at 100 mb or an altitude of about 16 kilometers. There the volumetric mass is close to 200 $g.m^{-3}$.

SIZE IN METERS OF CONDENSATION TRAILS FOR A WATER VAPOR OUTPUT OF $9.03.10^{3}$ $G.S^{-1}$ AS A FUNCTION OF THE DISTANCE MEASURED FROM THE SOURCE.*

Distance (km)	rs $g.g^{-1}$ / Persistence (seconds)	10^{-3}	10^{-4}	10^{-5}	5.10^{-6}
2	3,3	6	8	10	11
7,2	12	9	19	27	30
12	20	0	26	38	43
15	25	clear	29	44	50
40	66	clear	63	90	106
66	110	clear	0	128	156
81	135	clear	clear	150	187
198	330	clear	clear	232	350
360	600	clear	clear	0	450
600	1 000	clear	clear	clear	490
720	1 200	clear	clear	clear	350
810	1 350	clear	clear	clear	0

Distances corresponding to zero constitute maximum estimates of probable lengths of the condensation trails.

*commas represent decimal points

Except for the last column of this table (saturation mixture ratio rs = 5.10^{-6} $g.g^{-1}$), the influence of the natural water vapor content (r = 3.10^{-6} $g.g^{-1}$) [2] can be ignored. By performing the same kinds of calculations, it can be predicted that after 18 minutes (630 km), the maximum concentration contribution caused by the emission of one aircraft will be smaller than this natural content, and the "4.3 σ" size will be 1,100 m.

Three categories of conclusions can be derived from this first fundamental /44 and preliminary work.

In the first place, it must be stressed that all these calculations were carried out without taking any account of the dissociation and dispersion phenomena of the various products under discussion. For water vapor, for example, it is certain that the lack of precipitation in the stratosphere can result in a small dispersion. However, various other processes occur. Consequently, all the indicated numerical values which indicate favorable conditions (rapid return to conditions close to normal, favorable dimensions of the condensation trails) certainly represent underestimated values. Additional studies will have to be made to investigate this point.

Secondly, we should note that the orders of magnitude of the values found for the dimensions of the condensation trails represent a good test of the validity of the method proposed to attack the problem, in spite of the uncertainties which exist and even taking into account the fact that values obtained are underestimates, as discussed above.

Finally, just as for any method of this type, it is clear that a valid test of the method will be obtained by full scale "in situ" verifications within a region of the atmosphere which has been relatively little explored. These tests will be done by "accompanying aircraft" which will perform direct measurements of pollutant and tracer concentrations, as well as specific meteorological measurements.

Remarks

For time periods of about 10 years, the calculations should be made on another basis, because as far as the horizontal dimensions are concerned, the earth's atmosphere does not represent an infinite reservoir (additional accumulation effect).

Also, the spherical effects were ignored. They certainly can be ignored during the initial time periods, but should be considered in the further calculations, especially for the longer periods.

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REFERENCES

1. Doury, A. Une méthode de calcul pratique et générale pour la prévision numérique des pollutions véhiculées par l'atmosphère (A Practical and General Calculation Method for Numerical Prediction of Pollutants Transported by the Atmosphere). Report C.E.A. R 4280, 1972.

2. Reiter, E.R. Atmospheric Transport Processes, Part 2, Chemical Tracers. U.S.A.E.C. Division of Technical Information, 1971.

3. Sissenwine, N., D.D. Grantham and H.A. Salmela. Mid-Latitude Humidity to 32 km. Journal of the Atmospheric Sciences, Vol. 25, 1968, pp. 1129, 1140.

4. OACI - SSTP III WP 44 (Point 6 of the order of the day). 3rd Conference, Montreal, September, 1971.

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